

Numerical Renormalization Group for the sub-ohmic spin-boson model: A conspiracy of errors

Matthias Vojta

Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

(Dated: January 25, 2012)

The application of Wilson's Numerical Renormalization Group (NRG) method to dissipative quantum impurity models, in particular the sub-ohmic spin-boson model, has led to conclusions regarding the quantum critical behavior which are in disagreement with those from other methods and which are by now recognized as erroneous. The errors of NRG remained initially undetected because NRG delivered an internally consistent set of critical exponents satisfying hyperscaling. Here we discuss how the conspiracy of two errors – the Hilbert-space truncation error and the mass-flow error – could lead to this consistent set of exponents. Remarkably, both errors, albeit of different origin, force the system to obey naive scaling laws even when the physical model violates naive scaling. In particular, we show that a combination of the Hilbert-space truncation and mass-flow errors induce an artificial non-analytic term in the Landau expansion of the free energy which dominates the critical behavior for bath exponents $s < 1/2$.

PACS numbers: 05.30.Cc, 05.30.Jp

I. INTRODUCTION

The Numerical Renormalization Group method,^{1,2} originally developed¹ by Wilson for the Kondo model and subsequently applied to a variety of impurity models with fermionic baths, was generalized in Refs. 3,4 to the case of bosonic baths with an eye towards dissipative impurity models. In particular, it has been applied to the spin-boson model,⁵

$$\mathcal{H}_{\text{SB}} = -\frac{\Omega}{2}\sigma_x + \frac{\epsilon}{2}\sigma_z + \frac{\sigma_z}{2} \sum_i \lambda_i (b_i + b_i^\dagger) + \sum_i \omega_i b_i^\dagger b_i \quad (1)$$

where $\sigma_z = \pm 1$ are the local impurity states with bias ϵ , Ω is the tunneling rate, and the $\omega_i > 0$ and λ_i are the frequencies and coupling constants of the bath oscillators. The bath is completely specified by its propagator at the “impurity” location

$$\Gamma(\omega) = \sum_i \frac{\lambda_i^2}{\omega + i0^+ - \omega_i} \quad (2)$$

whose spectral density $J(\omega) = -\text{Im} \Gamma(\omega)$ is commonly parameterized as

$$J(\omega) = 2\pi \alpha \omega_c^{1-s} \omega^s, \quad 0 < \omega < \omega_c, \quad s > -1 \quad (3)$$

where the dimensionless parameter α characterizes the dissipation strength, and ω_c is a cutoff energy. The value $s = 1$ represents the case of ohmic dissipation. For $0 < s \leq 1$, the spin-boson model (1) displays a quantum phase transition (QPT) between a delocalized and a localized phase, reached for small and large α , respectively.³⁻¹⁵

NRG has enabled detailed investigations of this QPT. While statistical-mechanics arguments^{8,10,16} suggest that this transition is in the same universality class as the thermal phase transition of the one-dimensional (1d) Ising model with $1/r^{1+s}$ long-range interactions, initial

NRG results⁷ were in disagreement with this quantum-to-classical correspondence (QCC). In particular, NRG delivered s -dependent critical exponents which obeyed hyperscaling for all $0 < s < 1$. Those exponents agreed with the ones of the Ising model for $s > 1/2$, but disagreed for $s < 1/2$ where the Ising model is above its upper-critical dimension and displays mean-field behavior without hyperscaling.^{17,18} This apparent violation of QCC prompted further numerical investigations. Quantum Monte Carlo (QMC)¹⁰ and exact-diagonalization¹¹ studies led to the opposite conclusion, namely that the critical behavior of the spin-boson model for $s < 1/2$ is classical and of mean-field type.

Meanwhile, two different errors of the NRG method have been identified,¹⁹ which can be held responsible for incorrect results regarding critical properties. These two errors are the Hilbert-space truncation error, arising from the fact that the infinite Hilbert space of each bath harmonic oscillator needs to be truncated to N_b local states, and the mass-flow error, which is rooted in the iterative diagonalization procedure of NRG and leads to an effective shift of model parameters along the NRG run. The mass-flow error has been discussed in some detail in Ref. 20 where it has been shown to give rise to an incorrect exponent x , describing the thermal divergence of the susceptibility at criticality. Ref. 20 also implemented a recipe to correct the mass-flow error which then allowed to recover the mean-field value $x = 1/2$ for $s < 1/2$. The problem of Hilbert-space truncation has been solved in Ref. 13, by employing an optimized boson basis within a variational matrix-product-state approach on the Wilson chain. Applied to the spin-boson model with $s < 1/2$, this method not only delivered the expected mean-field values for the order-parameter exponents β and δ if the variational bosonic Hilbert space is taken to be (effectively) infinite, but also showed that artificially restricting the Hilbert space causes a crossover at small energies to the erroneous non-mean-field behavior of NRG.

The shortcomings of NRG have independently become clear in studies of dissipative anharmonic-oscillator models: These models are in one-to-one correspondence with a 1d Ising ϕ^4 theory with $1/r^{1+s}$ interactions and must therefore display a mean-field transition for $s < 1/2$. Nevertheless, standard NRG delivered²⁰ the same non-mean-field exponents as for the spin-boson model.

Together, these developments show that the initial NRG results⁷ were incorrect and that the QCC is fulfilled for the sub-ohmic spin-boson model. However, it has remained a puzzle *why and how* the NRG could produce an internally consistent set of exponents which moreover obeyed hyperscaling. This question is of obvious relevance for further applications of NRG. It is the purpose of the present paper to close this gap. We discuss Hilbert-space truncation in some detail, showing that the combination of Hilbert-space truncation and mass flows acts like a non-analytic term in the Landau expansion of the free energy. At criticality, this in turn forces the system to effectively remain locked at the upper-critical dimension for all $s \leq 1/2$. As a result, a set of “trivial” exponents with hyperscaling properties is obtained. While Hilbert-space truncation and mass flow may be thought of as independent sources of error, their effects are intertwined: As we argue below, the non-analytic term in the Landau expansion can be understood in terms of a *truncated mass flow*.

We note that recent papers^{21–23} insist on the breakdown of QCC for the spin-boson model. However, the concrete numerical results obtained in Refs. 21,23 are fully consistent with the scenario proposed here, as will be discussed below. Moreover, the objections raised against QCC in Ref. 22 do not apply. Hence, we believe the interpretation given in Refs. 21–23 is incorrect.

A. Outline

The remainder of the paper is organized as follows: Sec. II summarizes the spin-boson model, together with the standard derivation of its QCC via a Feynman path integral. It then reviews the properties of the resulting ϕ^4 theory – whose language will be heavily used in the paper – in particular the mean-field regime of $s < 1/2$ where Landau theory applies. Last but not least, Sec. II proposes that supplementing the field theory by a certain non-analytic term yields exactly the non-mean-field exponents seen in NRG – this non-analytic term will be derived and discussed in the remainder of the paper. Sec. III dives into technical details of NRG, by repeating and extending the discussion of the mass-flow error as given in Ref. 20 – this includes sub-leading corrections as addressed in Ref. 23. Finally, Sec. IV is devoted to the Hilbert-space truncation error and the truncated mass flow. It will highlight the crossover scales induced by the truncation and their influence on physical observables. A general discussion of NRG and its applicability to mean-field critical phenomena closes the paper.

II. SPIN-BOSON MODEL AND FIELD THEORY

On general grounds, one expects that the quantum phase transition in the spin-boson model can be described by a field theory for an Ising (i.e. real scalar) order parameter $\phi(\tau)$, where $\langle \phi \rangle$ corresponds to the local magnetization $\langle \sigma_z \rangle$.

A. Derivation

Such a field theory can be derived from the Feynman path-integral representation²⁴ of the partition function of \mathcal{H}_{SB} . One starts with a Trotter decomposition of the imaginary time axis into N intervals of length $\Delta\tau = \beta/N$. The operators $\exp(-\mathcal{H}_{\text{SB}}\Delta\tau)$ are then evaluated by inserting identity operators in terms of the eigenstates of σ_z , with eigenvalues $S = \pm 1$, and the bath-oscillator positions, q_i , for each time slice k . (Utilizing coherent states is not necessary, as \mathcal{H}_{SB} contains distinguishable objects only.²⁵) One arrives at:

$$\begin{aligned} \mathcal{S} = & - \sum_{k=1}^N \left[\frac{1}{2} \ln \coth(\Omega \Delta\tau) \right] S_k S_{k+1} \\ & + \sum_{k=1}^N \sum_i \left[\lambda_i \sqrt{m_i \omega_i} \Delta\tau S_k q_{k,i} \right. \\ & \left. + \frac{m_i}{2} \frac{(q_{k,i} - q_{k-1,i})^2}{\Delta\tau} + \Delta\tau \frac{m_i}{2} \omega_i^2 q_{k,i}^2 \right] \end{aligned} \quad (4)$$

where m_i are the masses of the bath oscillators, and the limit $\Delta\tau \rightarrow 0$ has to be taken at the end as usual.²⁴ Note that the action of σ_x in \mathcal{H}_{SB} has been evaluated directly. The oscillator bath is best treated in Fourier (i.e. frequency) space. Defining

$$\bar{S}_n = \frac{1}{\sqrt{N}} \sum_k e^{-2\pi i n k / N} S_k \quad (5)$$

for integer wavenumbers $n = 0, \dots, N-1$ and using the explicit form of the spectral density (3), one finds for the bath term the exact result:

$$\mathcal{S}_b = \sum_n \bar{S}_n \bar{S}_{-n} \pi \alpha \frac{(\omega_c \Delta\tau)^{1-s}}{\sin(\pi s / 2)} \left| 2 \sin \frac{\pi n}{N} \right|^s \quad (6)$$

The integrals in partition function involving the bath-oscillator coordinates are Gaussian, such that the bath oscillators can be integrated out exactly.²⁶ After transforming back to real space (i.e. time) the full action takes the form

$$\begin{aligned} \mathcal{S} = & - \sum_{k=1}^N \left[\frac{1}{2} \ln \coth(\Omega \Delta\tau) \right] S_k S_{k+1} \\ & + \frac{1}{2} \sum_{kk'} K(k-k') (S_k - S_{k'})^2. \end{aligned} \quad (7)$$

The bosonic bath thus generates a long-ranged self-interaction in imaginary time, with the long-distance behavior

$$K(k-k') = \alpha\Gamma(1+s)(\omega_c\Delta\tau)^{1-s} \frac{1}{(k-k')^{1+s}}, \quad (8)$$

valid for $1 \ll |k-k'| \ll N$. The representation (7) is real and free of a Berry-phase term.²⁵

At this stage, one may decide to interpret the S_k (for fixed finite $\Delta\tau$) as discrete spins, which form an Ising chain with long-range interactions. Its thermodynamic limit is obtained as $\beta \rightarrow \infty$, and one can show that the long-distance properties are independent of $\Delta\tau$. (This is somewhat non-trivial, as the nearest-neighbor coupling in (7) diverges as $\Delta\tau \rightarrow 0$, while the long-range coupling vanishes in the same limit.) Speculations that the limits $\Delta\tau \rightarrow 0$ and $\beta \rightarrow \infty$ might not commute⁷ have turned out to be unwarranted, as has been shown by explicit numerical computations.¹⁰ The phase transition in this Ising model itself is described by a continuum ϕ^4 theory with long-range interactions.¹⁷

Alternatively, one may depart from Eq. (4) and relax the hard-length constraint on the Ising variables. Assuming a slowly varying Ising order-parameter field ϕ then allows to obtain a continuum theory with finite coefficients, which is – of course – the same ϕ^4 theory as obtained for the discrete Ising model.

This ϕ^4 theory reads

$$\mathcal{S} = \int \frac{d\omega}{2\pi} (m_0 + |\omega|^s) |\phi(i\omega)|^2 + \int d\tau [u\phi^4(\tau) + \bar{\epsilon}\phi(\tau)] \quad (9)$$

the continuous frequency integral has to be replaced by a Matsubara sum for $T > 0$. The field ϕ has been re-scaled such that the prefactor of the $|\omega|^s$ term equals unity, and $\bar{\epsilon} \propto \epsilon$ represents the field conjugate to the order parameter. In Eq. (9) an increase of the (bare) mass parameter m_0 corresponds to a decrease in the dissipation strength α , with the critical point located at $m_0 = m_c$ or $\alpha = \alpha_c$.

By universality arguments, the same field theory describes a dissipative anharmonic oscillator

$$\begin{aligned} \mathcal{H}_{\text{DHO}} = & \Omega a^\dagger a + \frac{\epsilon}{2}(a + a^\dagger) + U n_a(n_a - 1) \\ & + \frac{1}{2} \sum_i \lambda_i (a + a^\dagger)(b_i + b_i^\dagger) + \sum_i \omega_i b_i^\dagger b_i, \end{aligned} \quad (10)$$

where $\Omega > 0$ is the bare “impurity” oscillator frequency, $n_a = a^\dagger a$, and U parameterizes the anharmonicity. For $U = \infty$, \mathcal{H}_{DHO} is equivalent to \mathcal{H}_{SB} , because all impurity states except $n_a = 0, 1$ are projected out. In the opposite limit of small U the interaction term of \mathcal{H}_{DHO} (10) is expected to follow the same RG flow as does u in \mathcal{S} (9).

B. Critical exponents

The field theory (9) can be utilized to calculate critical exponents, with the following definitions:

$$\begin{aligned} \phi(\alpha > \alpha_c, T = 0, \epsilon = 0) & \propto (\alpha - \alpha_c)^\beta, \\ \chi(\alpha < \alpha_c, T = 0) & \propto (\alpha_c - \alpha)^{-\gamma}, \\ \phi(\alpha = \alpha_c, T = 0) & \propto |\epsilon|^{1/\delta}, \\ \chi(\alpha = \alpha_c, T) & \propto T^{-x}, \\ \chi''(\alpha = \alpha_c, T = 0, \omega) & \propto |\omega|^{-y} \text{sgn}(\omega), \end{aligned} \quad (11)$$

where $\phi = \langle \phi \rangle$ and $\chi = d\phi/d\epsilon$. The last equation describes the dynamical scaling of χ .

The ϕ^4 theory (9) has been analyzed in detail in Ref. 17. Power counting yields the scaling dimensions at criticality:

$$\begin{aligned} \dim[\phi(\tau)] &= (1-s)/2, \\ \dim[u] &= 1 - 4\dim[\phi(\tau)] = 2s - 1, \end{aligned} \quad (12)$$

i.e., the system is above (below) its upper-critical dimension for $s < 1/2$ ($s > 1/2$). Consequently, the transition is controlled by a Gaussian fixed point for $s < 1/2$, with critical exponents

$$\beta_{\text{MF}} = 1/2, \quad \gamma_{\text{MF}} = 1, \quad \delta_{\text{MF}} = 3, \quad \nu_{\text{MF}} = 1/s, \quad (13)$$

where the s dependence of the correlation-length exponent ν reflects the influence of the long-range interactions. Moreover, the exponents x and y , related to the finite-size-scaling and anomalous decay exponents of the classical Ising model, are different:

$$x_{\text{MF}} = 1/2, \quad y_{\text{MF}} = s. \quad (14)$$

In contrast, for $s > 1/2$ the exponents take non-trivial values. Hyperscaling allows to deduce a few exact results, given that $y = s$ is known to be exact:^{18,27}

$$x_{\text{hyp}} = y_{\text{hyp}} = s, \quad \delta_{\text{hyp}} = \frac{1+s}{1-s}. \quad (15)$$

C. Temperature-dependent mass and susceptibility

As a prerequisite for the following considerations, we now explicitly derive the temperature dependence of the (renormalized) order-parameter mass at criticality, which is related to the susceptibility by $1/\chi(T) = m(T)$.

Below the upper-critical dimension, i.e., for $s > 1/2$, naive scaling applies. Given the zero-temperature form of the critical propagator $1/G_\phi \propto \omega^s$, the interaction-induced mass at criticality has to scale as $m(T) \propto T^s$, which yields $x = s$ as stated above.

In contrast, in the mean-field regime of $s < 1/2$, $m(T)$ can be obtained in lowest-order perturbation theory in u . The tadpole diagram at criticality evaluates to

$$\Sigma_1 = uT \sum_j \frac{1}{|\omega_j|^s + b\omega_j^2 + m(T)} \quad (16)$$

where $\omega_j = 2\pi jT$ are Matsubara frequencies and $b\omega_j^2$, representing the short-range piece of the interaction, has been included for convergence. The temperature-dependent piece, $\Sigma_1(T) - \Sigma_1(0) = m(T)$, can be obtained by simple scaling analysis. Assuming $m(T) = aT^x$ we find

$$aT^x = uT^{1-x} \left(\sum_j \frac{1}{|2\pi j|^s T^{s-x} + a} - \int \frac{dj}{|2\pi j|^s T^{s-x}} \right) \quad (17)$$

For $x > s$ and small T the right-hand side is dominated by the $j = 0$ piece of the sum and hence approaches a constant as $T \rightarrow 0$. Demanding the temperature power laws on both sides of Eq. (17) to match, we obtain $x = 1/2$ as expected¹⁷ (which indeed fulfills $x > s$).

The calculation shows that it is mandatory to include the mass self-consistently into the internal propagator of the tadpole diagram; this is different from the situation in ϕ^4 theories with short-ranged interactions where the tadpole diagram with bare propagator would be sufficient to determine the shift exponent.

D. Field theory with NRG errors

Our central result is that the errors of NRG induce extra non-analytic mass terms in the order-parameter field theory:

$$\mathcal{S}_{\text{err}} = \int d\tau \phi^2(\tau) \left[vT^s + w|\langle\phi\rangle|^{2s/(1-s)} \right], \quad (18)$$

with v and w depending on parameters of the NRG algorithm. The first term is a consequence of the mass flow, as discussed in Ref. 20 and summarized in Sec. III below. It is responsible for the incorrect result $x = s$ found using NRG for $s < 1/2$. The second term originates from Hilbert-space truncation, with the prefactor w scaling with the number N_b of bosons as $w \propto N_b^{-s/(1-s)}$. It will be derived in detail in Sec. IV.

Let us discuss the effect of the second term on critical exponents. Approximating $\phi(\tau)$ as static in $\mathcal{S} + \mathcal{S}_{\text{err}}$ and setting $T = 0$ leads to a Landau free energy

$$F(\phi) = \bar{\epsilon}\phi + m\phi^2 + w|\phi|^{2/(1-s)} + u\phi^4. \quad (19)$$

It is important to note that fluctuation corrections to this mean-field picture arise from the quartic u term only (as w is not an interaction), and hence will influence the critical behavior only for $s > 1/2$, where moreover $2/(1-s) > 4$ and hence the w term is subleading. In contrast, for $s < 1/2$ simply minimizing $F(\phi)$ (19) is sufficient to calculate the zero-temperature exponents. For $w = 0$ this of course results in $\beta_{\text{MF}} = 1/2$ and $\delta_{\text{MF}} = 3$. However, a non-zero w term dominates over the quartic u term for $s < 1/2$, and minimizing $F(\phi)$ then gives

$$\beta = \frac{1-s}{2s}, \quad \delta = \frac{1+s}{1-s}, \quad (20)$$

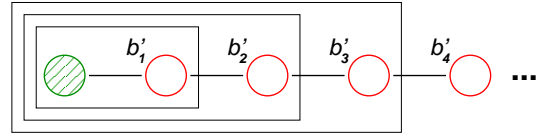


FIG. 1: (Color online) Structure of the NRG Hamiltonian, with the bath represented by a semi-infinite Wilson chain, with bath operators b'_n . The boxes indicate the iterative diagonalization scheme.

which are exactly the exponents observed⁷ in NRG! The equation of state derived from (19) is also consistent with the comprehensive scaling analysis of NRG results at different N_b performed in Ref. 28.

In the remainder of the paper, we discuss the errors of the bosonic NRG and the consequences of Eq. (18) in detail.

III. NRG AND MASS FLOW

The mass-flow problem of the bosonic NRG has been investigated in Ref. 20. Here we shall summarize the discussion and also provide an analysis of certain subleading corrections.

Within the NRG algorithm, the bath is represented by a semi-infinite (“Wilson”) chain, Fig. 1, such that the impurity is coupled to the first site of the chain only, and the local density of states at this first site is a discrete approximation to the bath density of states.^{1,2} Due to the logarithmic discretization, the site energies ε_n and hopping matrix elements t_n decay exponentially along the chain according to $\omega_c \Lambda^{-n+1}$, where Λ is the discretization parameter. We define a Hamiltonian \mathcal{H}_n for the impurity plus the first n sites of the Wilson chain, and we denote by $\Gamma_n(\omega)$ the corresponding propagator at the impurity site of this n -site bath. Then, \mathcal{H}_∞ with bath $\Gamma_\infty(\omega)$ is the discretized version of the original problem.

NRG proceeds by iteratively diagonalizing the Hamiltonian: First, \mathcal{H}_1 is diagonalized and the lowest N_s eigenstates are kept. Then, the next bath site is added to form \mathcal{H}_2 , the new system is diagonalized, and again the lowest N_s eigenstates are kept (which are approximations to the lowest states of \mathcal{H}_2). As the characteristic energy scale of the low-lying part of the eigenvalue spectrum decreases by a factor of Λ in each step, this process is repeated until the desired lowest energy is reached. Thermodynamic observables at a temperature $T_n = \omega_c \Lambda^{-n+1}/\bar{\beta}$ are typically calculated via a thermal average taken from the eigenstates at NRG step n . Here, $\bar{\beta}$ is a parameter of order unity which is often chosen as $\bar{\beta} = 1$.

A. Mass-flow error

The iterative diagonalization procedure implies that, at NRG step n , the chain sites $n+1$, $n+2$, ... have

not yet been taken into account, i.e., the effect of those sites does not enter thermodynamic observables at temperature T_n . The “missing” sites imply a missing contribution to the real part of the bath propagator. As detailed in Ref. 20, the zero-frequency value of this missing real part, $\text{Re}(\Gamma_\infty - \Gamma_n)(\omega = 0)$, scales as $(\bar{\beta}T_n)^s$ for a power-law bath spectrum, Eq. (3). In the field-theory language, the missing real part implies a temperature-dependent variation of the order-parameter mass. This is most clearly seen for the dissipative oscillator model in Eq. (10) where $\text{Re}\Gamma(\omega = 0)$ directly renormalizes the oscillator frequency, $\Omega \rightarrow \Omega + \text{Re}\Gamma(\omega = 0)$ at $U = 0$ (note that $\text{Re}\Gamma(\omega = 0) < 0$). Similarly, for the spin-boson model it is clear that the missing real part effectively leads to a temperature-dependent variation of model parameters. Provided that the spin-boson model renormalizes to the same ϕ^4 field theory as the dissipative oscillator, as shown in Sec. 4, it is clear that this variation is in the ϕ^4 mass.

Thus, the mass-flow error generates an artificial mass contribution $m_a = vT^s$ – this is the first term in \mathcal{S}_{err} (18). The prefactor v scales as $\bar{\beta}^s$, but also depends on the model and parameter regime under consideration (note that the mapping of the microscopic \mathcal{H} to the field theory involves coarse graining). Moreover, interaction effects will generate subleading contributions to m_a , see below.

B. Temperature dependence of χ in the presence of mass flow

As derived in Sec. II C, the irrelevant interaction u leads to an order-parameter mass $\propto T^{1/2}$ along the flow towards the Gaussian fixed point for $s < 1/2$. Consequently, the physical susceptibility follows $\chi \propto T^{-1/2}$ (Ref. 17). However, the artificial mass $m_a \propto T^s$ dominates the physical mass at low T , leading to the unphysical result $1/\chi \propto T^s$ – which happens to coincide with the physical result for an interacting fixed point with hyperscaling.

Considering the results in Ref. 23, it is worth evaluating the subleading correction to the mass-flow-determined $m_a = vT^s$. This piece, $m_2(T)$, is now arising from the quartic interaction and can be evaluated in lowest-order perturbation theory. In analogy to Eq. (16) we need to evaluate $\Sigma_1(T) - \Sigma_1(0) = m_2(T)$, with

$$\Sigma_1 = uT \sum_n \frac{1}{|\omega_n|^s + b\omega_n^2 + vT^s + m_2(T)} \quad (21)$$

where the propagator now contains *both* the artificial and the interaction-generated mass contribution. Assuming $m_2(T) = v_2T^{x_2}$ with $x_2 > s$, the m_2 term in the internal propagator is subleading. Consequently, the equation determining m_2 reads

$$v_2T^{x_2} = uT \left(\sum_j \frac{1}{(|2\pi j|^s + v)T^s} - \int \frac{dj}{|2\pi j|^s T^s} \right) \quad (22)$$

and one immediately arrives at $x_2 = 1 - s$. Hence, the presence of the artificial mass modifies the interaction-generated mass.²⁹ Indeed, the NRG results for $\chi(T)$ for both the spin-boson model²³ and the dissipative anharmonic oscillator²⁰ are consistent with $x_2 = 1 - s$ and thus in line with the above calculation. The calculation falsifies the claim of Ref. 23 that $x_2 > 1/2$ would be incompatible with the mass-flow scenario.

C. Mass-flow correction

Ref. 20 proposed an empirical algorithm to cure the mass-flow problem. This is based on compensating the NRG-induced mass flow by including an explicit temperature-dependent term, with coefficient κT^s , in the Hamiltonian which shifts the critical point similar to the effect of $\text{Re}\Gamma$. For the spin-boson model, the natural choice is to add a temperature-dependent piece to the tunneling matrix element Ω . In this procedure, κ remains a free parameter, and Ref. 20 proposed to adjust its value at criticality such that the unphysical T^s piece in $1/\chi$ is removed. This algorithm, dubbed NRG*, was shown to work well and to yield the expected mean-field behavior $1/\chi \propto T^{1/2}$ at low temperature for $s < 1/2$ whereas the T^s behavior was stable for $s > 1/2$. Therefore, the QCC for the exponent x has been confirmed by NRG*.

Ref. 23 recently questioned this result, based on the observation that $1/\chi(T)$ from NRG*, which follows $T^{1/2}$ at low T , displays an unusual *downward*-deviation from this law at higher T (see Figs. 7b and 8b of Ref. 20). Ref. 23 claimed that this would reflect an underlying temperature power law with exponent smaller than $1/2$, then supposedly inconsistent with mean-field behavior. Here we argue instead that the downward-deviation can be straightforwardly understood in terms of the mass flow and its compensation. As explained in Ref. 20, the mass-flow correction term with fixed κ only compensates for the mass flow near a specific fixed point, and different fixed points would require different κ . In other words, if the proper κ_0 for the low-temperature fixed point has been chosen, then this will compensate the artificial mass only to leading order, but a subleading term will be left over. For the spin-boson model, one can easily understand the sign of the subleading term by noting that NRG* produces an overcompensation of the mass flow at elevated temperatures or energies: At high energies, $\text{Re}\Gamma$ influences the mass very little (note that it couples to σ_z^2 in Eq. (1) in the short-time limit). Then, at high energies, only the mass-flow correction is active, which leads to a downward correction of the mass. It is this downward correction that causes the downturn in $1/\chi(T)$. (We also note that the downturn does not correspond to a new power-law regime, contrary to the assertion of Ref. 23.) We conclude that the downturn in $1/\chi(T)$ is not physical, but instead related to the shortcomings of the simple mass-flow correction in NRG*. The

same downturn is observed when applying NRG* to the dissipative anharmonic oscillator with large U .

IV. NRG AND HILBERT-SPACE TRUNCATION

In this section, we discuss how the truncation of the bosonic Hilbert space at each site of the Wilson chain, i.e., using only the lowest N_b occupation-number eigenstates of the oscillator as basis, influences the evaluation of observables in the spin-boson model. In particular, we will explain how the non-analytic w term in the effective field theory (18) emerges.

Hilbert-space truncation is bound to become important if σ_z develops a finite expectation value, either inside the ordered phase or in an applied field ϵ . For a finite $\langle\sigma_z\rangle$, the bath oscillators will have a finite displacement $\langle x_n \rangle = \langle b_n^\dagger + b_n \rangle$. By considering the system at the localized fixed point, $\Delta = 0$, it is easy to show that – due to the logarithmic discretization scheme of NRG – $\langle x_n \rangle$ diverges in the low-energy limit for $s < 1$ according to $\epsilon_n^{(s-1)/2}$. This implies that the average boson numbers diverge as well:

$$\langle b_n^\dagger b_n \rangle \propto \langle \sigma_z \rangle^2 \epsilon_n^{s-1}. \quad (23)$$

Importantly, $\langle \sigma_z \rangle$ in this equation is a temperature-dependent quantity which thus depends on n as well, but will typically saturate below a temperature T_{sat} .

A. Truncated mass flow

Trivially, for $N_b = \infty$ there are no truncation effects, and $\langle b_n^\dagger b_n \rangle$ diverges in the low-energy limit $n \rightarrow \infty$. For any finite N_b , the divergence of $\langle b_n^\dagger b_n \rangle$ is cut-off at some n_{cut} , where $\langle b_n^\dagger b_n \rangle$ reaches a value of order $\mathcal{O}(N_b)$. In the NRG algorithm, n_{cut} corresponds to a cut-off energy or temperature given by $T_{\text{cut}} = \epsilon_{n_{\text{cut}}}$, below which truncation is relevant. From Eq. (23) we deduce $N_b \propto \langle \sigma_z \rangle^2 T_{\text{cut}}^{s-1}$ which yields

$$T_{\text{cut}} \propto N_b^{-1/(1-s)} |\langle \sigma_z \rangle|^{2/(1-s)}. \quad (24)$$

What happens below T_{cut} ? The sites of the Wilson chain with $n > n_{\text{cut}}$ no longer behave as free bosonic states with energy ϵ_n : The low-energy states of the shifted oscillators are missing, because the truncated basis of the lowest N_b occupation-number eigenstates is too small to accommodate them. Qualitatively, the energies of the oscillators with $n > n_{\text{cut}}$ are systematically shifted upwards. By Kramers-Kronig relations this implies that the corresponding real part, $\text{Re } \Gamma_n$, is modified into $\text{Re } \tilde{\Gamma}_n$ for $n > n_{\text{cut}}$, with $\text{Re } \tilde{\Gamma}_\infty$ not reaching $\text{Re } \Gamma_\infty$.

This is where the mass-flow effect comes into play. The artificial mass $m_a(T)$, given by $\text{Re}(\Gamma_\infty - \Gamma_n)$ from the “missing” part of the Wilson chain, will no longer decrease $\propto T^s$ below T_{cut} , but will instead approach a constant value m_{cut} dictated by $\text{Re}(\Gamma_\infty - \tilde{\Gamma}_\infty)$. This constant

can be easily estimated: Assuming that the oscillators with $n > n_{\text{cut}}$ are shifted to infinite energy, it is given by $m_{\text{cut}} = v T_{\text{cut}}^s$; corrections to this simple estimate will modify the prefactor, but not the power-law dependence on T_{cut} . These considerations imply that the artificial mass m_a will only flow very little below T_{cut} , i.e., the mass flow is truncated at T_{cut} .

Taking the mass-flow and truncated mass-flow contributions together, we arrive at an artificial mass term in the order-parameter theory, which scales as $[\max(T, T_{\text{cut}})]^s$. Accounting for different prefactors and inserting Eq. (24) we arrive at the non-analytic mass terms as postulated in Sec. IID above:

$$\mathcal{S}_{\text{err}} = \int d\tau \phi^2(\tau) \left[v T^s + w |\langle \phi \rangle|^{2s/(1-s)} \right], \quad (25)$$

where $w \propto N_b^{-s/(1-s)}$ vanishes as $N_b \rightarrow \infty$.

As mentioned in Sec. IID the non-analytic w term asymptotically dominates over the quartic u term for $s < 1/2$ in the mean-field equation of state, Eq. (19), such that it leads to the incorrect critical exponents (20) observed in NRG.

In the power-counting sense, the non-analytic w term is *marginal* for all s : Using Eq. (12) we have

$$\dim[w] = 1 - \frac{2}{1-s} \dim[\phi(\tau)] = 0. \quad (26)$$

The system is thus effectively locked at an upper-critical dimension. This explains why the NRG exponents (20) obey hyperscaling, but are nevertheless “trivial” in the sense that only simple fractions of s occur. (Note that logarithmic corrections do not occur, due to the absence of fluctuation effects from w .)

B. Example: Order-parameter exponent δ

To illustrate the above considerations, we now discuss explicitly the behavior of the magnetization at the critical point in a small applied field ϵ as function of temperature T , which yields the critical exponent δ according to $\epsilon \propto \phi^\delta$ as $T \rightarrow 0$ (where $\phi = \langle \sigma_z \rangle$).

We discuss the physical behavior of the ϕ^4 model (9) in the absence of systematic errors first. The leading temperature dependence of the magnetization stems from the temperature-induced order-parameter mass $m(T)$. In the mean-field regime of $s < 1/2$, this can be estimated from the equation of state:

$$0 = \epsilon + m(T)\phi + 3u\phi^3. \quad (27)$$

Since $m(T) \rightarrow 0$ as $T \rightarrow 0$, ϕ will saturate below T_{sat} , with $m(T_{\text{sat}}) \propto \phi^2(T=0)$. Using $m(T) \propto T^{1/2}$ and $\delta = 3$, valid in the mean-field regime, we obtain

$$T_{\text{sat}} \sim \epsilon^{4/3} \quad (s < 1/2). \quad (28)$$

This argument can be generalized to the non-mean-field regime of $s > 1/2$, using $m(T) \propto T^s$, leading to

$$T_{\text{sat}} \sim \epsilon^{2/(s\delta)} \quad (s > 1/2). \quad (29)$$

From Eq. (27) one also sees that, above T_{sat} , ϕ will follow $\phi \propto \epsilon/m(T)$.

Now we turn to the influence of the systematic NRG errors. This requires to discuss the relation between T_{sat} , the physical saturation temperature of ϕ , and T_{cut} , the temperature below which Hilbert-space truncation spoils the calculation.

First assume that $T_{\text{sat}} > T_{\text{cut}}$. Then the magnetization will have taken its $T = 0$ value $\phi \propto \epsilon^{1/\delta}$ already above T_{cut} . From Eq. (24) we deduce

$$T_{\text{cut}} \propto \epsilon^{2/[(1-s)\delta]} \quad (\text{if } T_{\text{sat}} > T_{\text{cut}}). \quad (30)$$

Comparing this with Eq. (29), we see that, for small ϵ , indeed $T_{\text{sat}} > T_{\text{cut}}$ consistently holds for $s > 1/2$. In such a case, we expect that the Hilbert-space truncation will not significantly influence the $T = 0$ value of ϕ . This is in contrast to $s < 1/2$, where the assumption $T_{\text{sat}} > T_{\text{cut}}$ is found to be violated.

Now let us discuss the case $T_{\text{sat}} < T_{\text{cut}}$, applying to $s < 1/2$, where Hilbert-space truncation will affect the impurity magnetization. First, note that the estimate of T_{sat} (28) needs to be modified due to the mass-flow error: $m(T) \propto T^s$ yields

$$T_{\text{sat}} \sim \epsilon^{2/(3s)} \quad (s < 1/2, \text{ mass flow}). \quad (31)$$

At T_{cut} , the magnetization can be estimated as $\phi \propto \epsilon/m(T_{\text{cut}})$. Again using $m(T) \propto T^s$ and combining this with Eq. (24) we have

$$\phi(T_{\text{cut}}) \propto \frac{\epsilon}{\phi(T_{\text{cut}})^{2s/(1-s)}} \quad (32)$$

and

$$T_{\text{cut}} \propto \epsilon^{2/(1+s)} \quad (s < 1/2, \text{ mass flow}). \quad (33)$$

As argued above, due to the truncated mass flow, m remains of order T_{cut}^s for all $T < T_{\text{cut}}$. Therefore Eq. (32) implies that

$$\phi \sim \phi(T_{\text{cut}}) \propto \epsilon^{(1-s)/(1+s)} \quad (34)$$

holds down to $T = 0$, resulting in the critical exponent $\delta = (1+s)/(1-s)$ as indeed observed.

The truncated mass flow is shown using NRG data in Fig. 2. For $s < 1/2$ the magnetization $\phi = \langle \sigma_z \rangle$ indeed increases down to T_{cut} , but stops to increase below T_{cut} – this proves both $T_{\text{sat}} < T_{\text{cut}}$ and $m(T) \approx \text{const}$ for $T < T_{\text{cut}}$. The latter reflects the advertised truncated mass flow and leads to incorrect scaling. In contrast, for $s > 1/2$ the magnetization saturates already above T_{cut} , indicating $T_{\text{sat}} > T_{\text{cut}}$ as argued above.

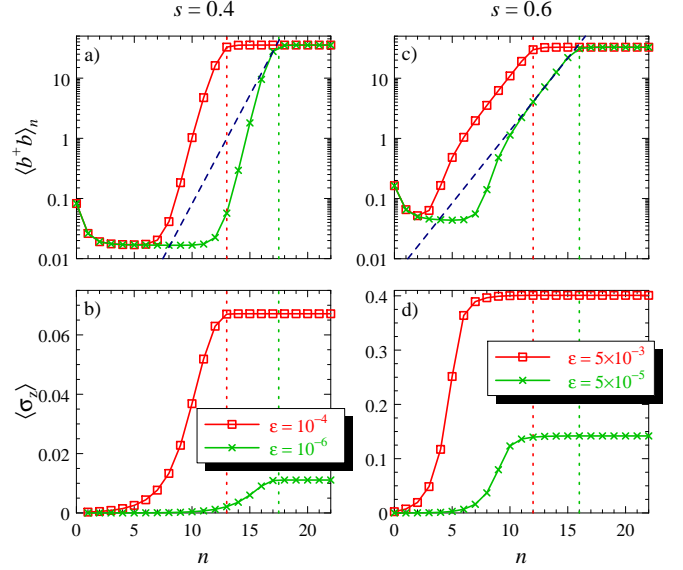


FIG. 2: (Color online) Evolution of the boson occupation number, $\langle b_n^\dagger b_n \rangle$, and the magnetization, $\langle \sigma_z \rangle$, in the spin-boson model at criticality in an applied field ϵ , as calculated along the NRG run with $\Delta = 1$, $\Lambda = 4$ and $N_b = 50$. a,b) For $s = 0.4$ ($\alpha_c = 0.0355465$), both quantities saturate at the same n , or equivalently, the same temperature T_{cut} (dotted vertical lines), illustrating that Hilbert-space truncation affects the magnetization. c,d) In contrast, for $s = 0.6$ ($\alpha_c = 0.06702411$) the magnetization saturates before T_{cut} is reached, and is thus unaffected by truncation. The dark dashed lines indicate a divergence $\langle b_n^\dagger b_n \rangle \propto \epsilon_n^{s-1}$ according to Eq. (23) – this is not realized for $s = 0.4$ because $\langle \sigma_z \rangle$ is never constant above T_{cut} , but applies to $s = 0.6$ in the interval $T_{\text{cut}} < T < T_{\text{sat}}$ where $\langle \sigma_z \rangle$ is constant.

Importantly, Fig. 2 illustrates the qualitative difference between $s < 1/2$ and $s > 1/2$ independent of the knowledge of the underlying field theory: Hilbert-space truncation limits the magnetization only for $s < 1/2$, where it consequently spoils the physical critical behavior.

Upon increasing the applied field ϵ for $s < 1/2$, T_{sat} (31) will increase faster than T_{cut} (33), such that the correct mean-field behavior is recovered at $T = 0$ for intermediate values of ϵ .¹⁹ This crossover is fully described by the equation of state

$$|\bar{\epsilon}| = \bar{w} N_b^{-s/(1-s)} \phi^{(1+s)/(1-s)} + 3u\phi^3 \quad (35)$$

obtained from minimizing (19) for $m = 0$, i.e., at criticality, and setting $w = \bar{w} N_b^{-s/(1-s)} (1-s)/2$. A comparison of this prediction with numerical data is shown in Fig. 3, with excellent agreement except for very small N_b where the continuum approximation w.r.t. N_b is not yet accurate.

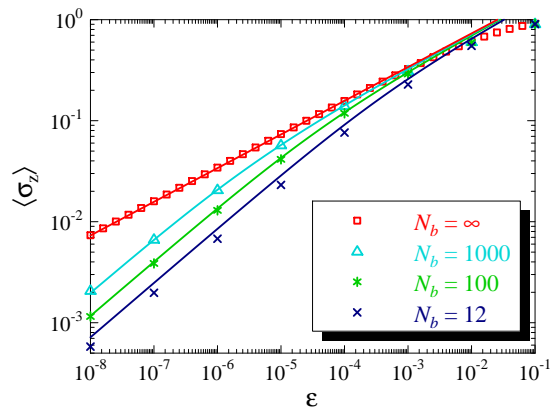


FIG. 3: (Color online) Effect of Hilbert-space truncation on the evaluation of the critical exponent δ in the spin-boson model for $s = 0.3$. The data points have been obtained using the variational matrix-product-state approach of Ref. 13 with parameters $\Lambda = 2$, $\Delta = 0.1$ where $\alpha_c = 0.0346142$; for small N_b results from standard NRG are identical up to minimal deviations. The lines show the crossover behavior according to the equation of state (35) with $\bar{w} = 1/50$ and $3u = 1/39$ – this gives an excellent description of the data for not too small N_b .

V. DISCUSSION

We have shown that mass flow, i.e., the fact that the order-parameter mass depends on the length n of the Wilson chain, is the source of all incorrect exponents obtained by NRG for the spin-boson model: (i) The incorrect finite-temperature exponent x arises because the rest of the chain is discarded when calculating finite-temperature observables at a temperature T_n . (ii) The incorrect zero-temperature exponents β and δ arise because the chain is effectively truncated at some magnetization-dependent n_{cut} where the diverging oscillator shifts can no longer be accommodated within the finite Hilbert space for each boson site. In the order-parameter field theory, (i) and (ii) can be captured as artificial non-analytic mass contributions, Eq. (18).

The fact that the resulting NRG exponents are internally consistent and obey hyperscaling can be rationalized by realizing that both errors of bosonic NRG can be associated with *stationarity* along the NRG flow. (A) The mass-flow error enforces the temperature-dependent renormalized mass to be stationary at criticality (which corresponds to naive scaling $m_a \propto T^s$). (B) The Hilbert-space truncation error cuts the divergence of the boson

occupation number, making it stationary. Thus, both errors force the NRG flow to show fixed-point behavior – in the NRG sense of stationarity of the many-body energies and states along the flow – in a situation where the correct physical RG flow does not show stationarity in the same sense. This applies both to the localized phase of the spin-boson model, where the boson number diverges along the Wilson chain, and to the flow towards the Gaussian critical point, where the true many-body level spacing goes to zero as $T \rightarrow 0$ because of the irrelevance of the quartic interaction.²⁰

This finally solves the puzzle: NRG produces incorrect exponents obeying hyperscaling because its algorithmic deficiencies force the NRG flow to be stationary, which implies naive scaling. One concludes that it is difficult with traditional NRG to describe critical phenomena which violate hyperscaling and are controlled by a dangerously irrelevant variable because in such a case the NRG flow will not be stationary near the physical RG fixed point³⁰ – this has been (partially) illustrated in Ref. 20. Algorithmic modifications, e.g. the variational matrix-product-state approach of Ref. 13, can in principle solve the problem.

The present insights show that NRG-based claims of violated QCC in other Ising-symmetric impurity models with sub-ohmic bosonic baths^{33,34} should be revisited. Also, implications for the calculation of dynamical properties^{35–38} need to be investigated. In bosonic impurity models with higher symmetries, QCC was found to be fulfilled for a rotor model,³⁹ but argued to be violated for XY-symmetric spin-boson¹³ and SU(2)-symmetric Bose-Kondo models.⁴⁰ These results suggest that the violation of QCC is related to the presence of multiple baths (or long-ranged interactions) which couple to different *non-commuting* impurity operators. Clearly, a deeper understanding of the relevant non-classical phase transitions is desirable.

Acknowledgments

We thank J. von Delft, K. Ingersent, S. Kirchner, Q. Si, N. Tong, and, in particular, S. Florens, R. Narayanan, and T. Vojta for discussions, and R. Bulla, J. von Delft, C. Guo, H. Rieger, N. Tong, and A. Weichselbaum for collaborations on related topics. We also thank C. Guo for providing the data in Fig. 3. This research has been supported by the DFG (FOR 960) and the GIF.

¹ K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

² R. Bulla, T. Costi, and T. Pruschke, Rev. Mod. Phys. **80**, 395 (2008).

³ R. Bulla, N. Tong, and M. Vojta, Phys. Rev. Lett. **91**, 170601 (2003).

⁴ R. Bulla, H.-J. Lee, N. Tong, and M. Vojta, Phys. Rev. B **71**, 045122 (2005).

⁵ A. J. Leggett, S. Chakravarty, A.T. Dorsey, M.P.A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).

⁶ S. Kehrein and A. Mielke, Phys. Lett. A **219**, 313 (1996).

- ⁷ M. Vojta, N. Tong, and R. Bulla, Phys. Rev. Lett. **94**, 070604 (2005).
- ⁸ M. Vojta, Phil. Mag. **86**, 1807 (2006).
- ⁹ K. Le Hur, P. Doucet-Beaupre, and W. Hofstetter, Phys. Rev. Lett. **99**, 126801 (2007).
- ¹⁰ A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. **102**, 030601 (2009).
- ¹¹ A. Alvermann and H. Fehske, Phys. Rev. Lett. **102**, 150601 (2009).
- ¹² H. Wong and Z.-D. Chen, Phys. Rev. B **77**, 174305 (2008).
- ¹³ C. Guo, A. Weichselbaum, J. von Delft, and M. Vojta, preprint arXiv:1110.6314.
- ¹⁴ S. Florens, D. Venturelli, and R. Narayanan, Lect. Notes Phys. **802**, 145 (2010).
- ¹⁵ A. W. Chin, J. Prior, S. F. Huelga, and M. B. Plenio, Phys. Rev. Lett. **107**, 160601 (2011).
- ¹⁶ V. J. Emery and A. Luther, Phys. Rev. B **9**, 215 (1974).
- ¹⁷ E. Luijten and H. W. J. Blöte, Phys. Rev. B **56**, 8945 (1997).
- ¹⁸ M. E. Fisher, S.-k. Ma, and B. G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
- ¹⁹ M. Vojta, N. Tong, and R. Bulla, Phys. Rev. Lett. **102**, 294904(E) (2009).
- ²⁰ M. Vojta, R. Bulla, F. Güttge, and F. B. Anders, Phys. Rev. B **81**, 075122 (2010).
- ²¹ S. Kirchner, Q. Si, and K. Ingersent, Phys. Rev. Lett. **102**, 166405 (2009).
- ²² S. Kirchner, J. Low Temp. Phys. **161**, 282 (2010).
- ²³ S. Kirchner, Q. Si, and K. Ingersent, preprint arXiv:1111.6623.
- ²⁴ J. W. Negele and H. Orland, *Quantum Many-Particle Systems*, Addison-Wesley (Reading), 1988.
- ²⁵ A representation of \mathcal{H}_{SB} using coherent spin states, and consequently an imaginary Berry phase, is possible as well.²² However, this by itself does not imply the invalidity of QCC, as both this coherent-state representation and the real representation of Sec. II A faithfully represent the physics of the quantum model.
- ²⁶ None of the objections in Sec. 2 of Ref. 22 applies.
- ²⁷ M. Suzuki, Prog. Theor. Phys. **49**, 424, 1106, 1440 (1973).
- ²⁸ Y.-H. Hou and N.-H. Tong, Eur. Phys. J. B **78**, 127 (2010); N.-H. Tong and Y.-H. Hou, preprint arXiv:1012.5615.
- ²⁹ Ref. 20 asserted that, in the presence of mass flow, the temperature dependence of the order-parameter mass for $s < 1/2$ follows $vT^s + v_2T^{1/2}$, with the second term representing the interaction-generated physical mass. This assertion was incorrect: As detailed in Sec. III, the interaction-generated mass is modified by the artificial mass, such that the correct behavior is $vT^s + v_2T^{1-s}$.
- ³⁰ The fermionic pseudogap Kondo model with bath exponent $r > 1$ provides an example for a phase transition above an upper-critical dimension, with hyperscaling violated, where NRG nevertheless works.³¹ This is related to the fact that the effective “Gaussian” theory is that of a level crossing, without dangerously irrelevant variables.³² The many-body level spectrum has a well-defined finite spacing even at the “Gaussian” fixed point.
- ³¹ C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B **57**, 14254 (1998).
- ³² M. Vojta and L. Fritz, Phys. Rev. B **70**, 094502 (2004); L. Fritz and M. Vojta, *ibid.* **70**, 214427 (2004).
- ³³ M. T. Glossop and K. Ingersent, Phys. Rev. Lett. **95**, 067202 (2005); Phys. Rev. B **75**, 104410 (2007).
- ³⁴ M. Cheng, M. T. Glossop, and K. Ingersent, Phys. Rev. B **80**, 165113 (2009).
- ³⁵ A. Chin and M. Turlakov, Phys. Rev. B **73**, 075311 (2006).
- ³⁶ F. B. Anders, R. Bulla, and M. Vojta, Phys. Rev. Lett. **98**, 210402 (2007).
- ³⁷ P. Nalbach and M. Thorwart, Phys. Rev. B **81**, 054308 (2010).
- ³⁸ S. Florens, A. Freyn, D. Venturelli, and R. Narayanan, Phys. Rev. B **84**, 155110 (2011).
- ³⁹ M. Al-Ali and T. Vojta, Phys. Rev. B **84**, 195136 (2011).
- ⁴⁰ L. Zhu, S. Kirchner, Q. Si, and A. Georges, Phys. Rev. Lett. **93**, 267201 (2004); S. Kirchner and Q. Si, preprint arXiv:0808.2647.